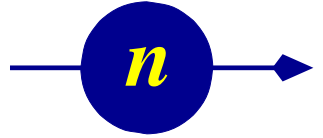




Technical University of Denmark



*McStas*



# CAMEA

## Concept and Science Case

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ÉCOLE POLYTECHNIQUE  
FÉDÉRALE DE LAUSANNE

## **Danish-Swiss Work Package 1: CAMEA**

### **Continuous Angular Multiple Energy Analysis Spectrometer**

#### **Report on Instrument Concept and Scientific Case**

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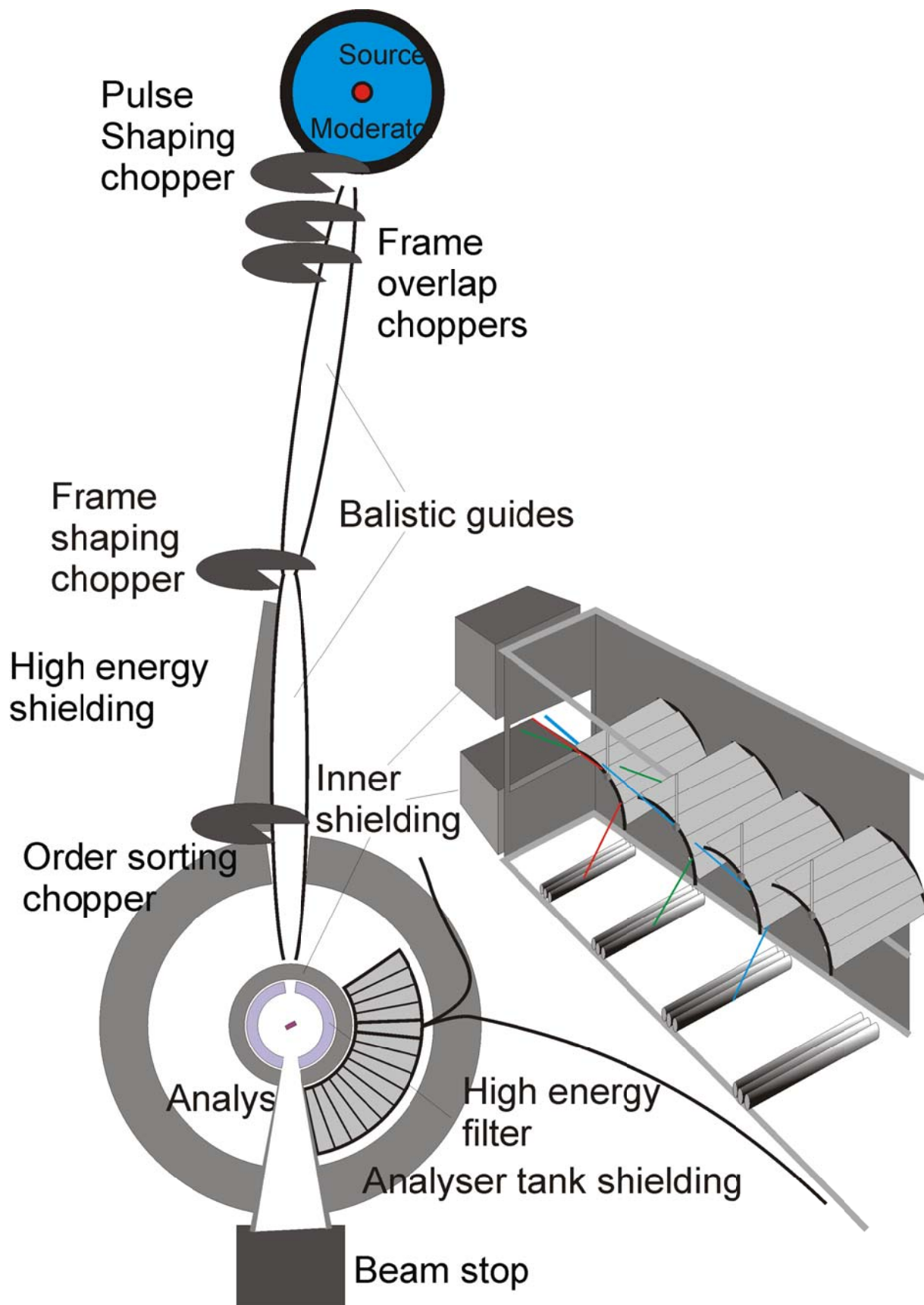
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## **Abstract**

This work unit proposes to construct a cold indirect geometry time of flight spectrometer for performing inelastic neutron scattering experiments optimized for optimal efficiency in the horizontal scattering plane at the European Spallation Source. A horizontal geometry is chosen for compatibility with performing neutron scattering experiments under extreme conditions. The instrument concept is called the Continuous Angular Multiple Energy Analysis Spectrometer, CAMEA. In this report we will outline the science case for CAMEA, highlighting the science that could be performed on CAMEA, the demand for an instrument of this type, as well as identifying the current and future technology in neutron scattering that can be utilized.

The basic concept of CAMEA is to maximize neutron count rates for scattering in the horizontal plane, with a quasi-continuous angular coverage of the scattered neutrons. High neutron detection efficiency will be obtained by using banks of concentric analysers placed behind each other, analysing different neutron energies of the scattered neutrons. Optimization of a horizontal scattering geometry has been chosen to be compatible with extreme sample environments and the ability to perform inelastic neutrons scattering studies. We will highlight how this provides a generation of advancement in inelastic neutron scattering under extreme environments, and what new possibilities for scientific studies CAMEA enables in inelastic neutron scattering.



Overview of the CAMEA instrument layout and the analyzer-detector concept, not to scale.

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# 1) Concept

## 1a) Motivation

Neutron spectroscopy is a particularly powerful technique in condensed matter research, particularly in the fields of correlated electron materials and quantum magnetism. It is a unique tool in allowing momentum and energy resolved information on magnetic excitations and fluctuations in studied materials. Recent developments in resonant inelastic x-rays (RIXS) scattering complement inelastic neutron scattering. RIXS can study magnetic excitations in materials of 100  $\mu\text{m}$  diameter to eV energies, but has several limitations in comparison to inelastic neutron scattering. The low energy x-rays required for RIXS have short penetration depths into materials, a problem for in-situ measurements. X-ray beam heating limits either the minimum achievable temperature to the order of several Kelvin or limits the maximum incident flux. Envisaged projects for the new RIXS spectrometers ERIXS at the ESRF (France), Centurion at NSLS-II (USA), spectrometers at the Diamond Light Source (UK), MAX IV (Sweden) and at other light sources, aim to achieve of the order of 5-10 meV energy resolution[1]. On the other hand cold neutron spectrometers can achieve energy resolutions below 50  $\mu\text{eV}$ , reaching temperatures down to 50 mK, and neutrons can readily penetrate complex sample environments. The main limitation of inelastic neutron scattering is counting statistics due to low neutron flux and weak scattering cross-sections, meaning samples need to be orders of magnitude larger than those used in x-ray experiments.

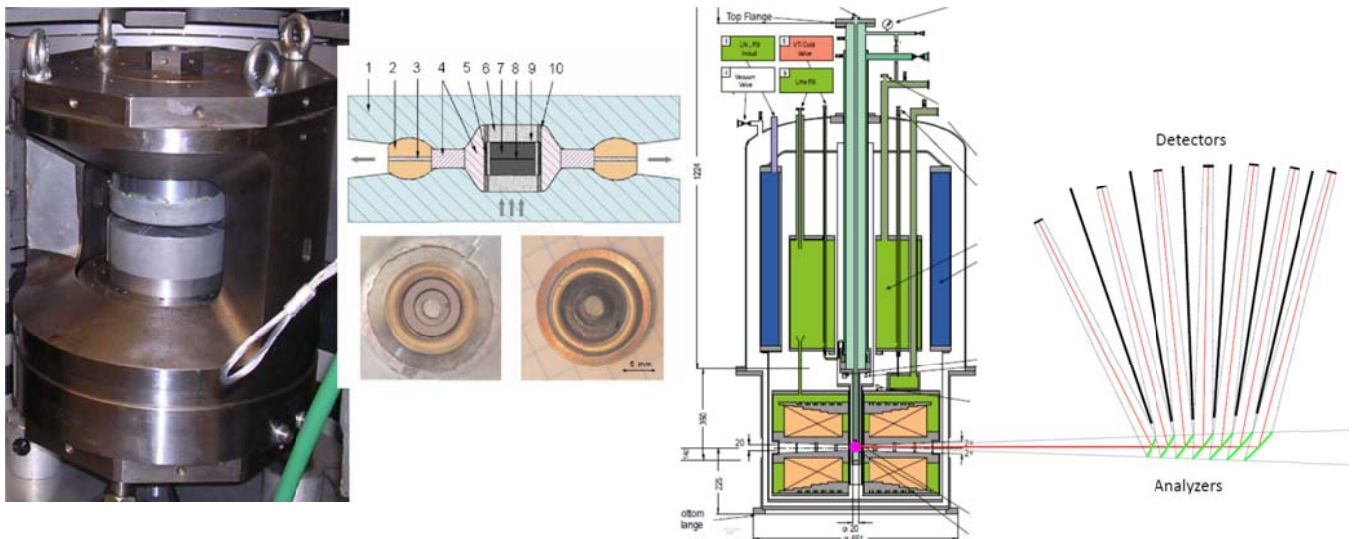


Figure 1: Left: A Paris-Edinburgh pressure cell that has a small vertical axis for neutrons. Centre: A diagram of a sample gasket inside a Paris-Edinburgh cell. Right: A diagram of a cryomagnet with restrictive vertical neutron access, alongside the main components of a CAMEA analyser setup. In this diagram the shielding tank around the analysers and detectors has been omitted for clarity, only neutrons that scattered into the solid angle of the analysers enter the shielding tank.

To understand the underlying physics of materials it is necessary to understand the different phases of these systems across the material's phase diagram. Studying the phase diagram of systems involve changing their properties by changing electronic doping level of the material, external or internal pressure, temperature, applying a magnetic or electric field on

the material, etc.. Changing a material's properties by changing doping level or changing the structure to introduce internal pressure necessarily alters the material being studied, opening up the question of whether effects are intrinsic to the underlying physics or extrinsic effects due to impurities in the material. Contrary to this, when an electronic phase diagram is studied by application of an external force, the sample quality is constant, and only intrinsic properties of the material vary. Examples of external forces that can be applied are high magnetic fields and high pressures. Furthermore the application of an external force can enable experimenters to tune systems into phases that cannot be found by sample growth, this allows experimenters to probe the emergent phenomena of new phases of matter. Using an applied external force therefore represents the cleanest way to study material phase diagrams, which in turn facilitates the realization of novel material states and investigating emergent phenomena.

The study of material phase diagrams by application of an external force in neutron scattering is limited by the achievable extreme sample environments, and the compatibility of these sample environments with neutron scattering instrumentation. The CAMEA concept is conceived as a neutron scattering instrument optimized to maximize counting efficiency in the horizontal scattering plane, a geometry that matches the performance required for performing inelastic neutron scattering under extreme conditions. To match the energy scale of the external forces that extreme environments can exert, plus the most desirable energy range and energy resolution for the science CAMEA can perform, CAMEA will be optimized for cold neutrons (2-25 meV). CAMEA's incident energy range will extend up to 80 meV to give access to the largest energy range that can be used by the CAMEA crystal analysers.

## **1b) Existing Spectrometers**

The so-called triple-axis-spectrometer (TAS), the invention of which gave Bertram Brookhouse the 1994 Nobel Prize, continues to be a primary workhorse of neutron spectroscopy. Its force is flexibility in measuring a selected point in  $(q, \omega)$  with high intensity. However, while focusing techniques allow many neutrons onto the sample, only a tiny fraction of the scattered neutrons are recorded.

The main development in neutron spectroscopy is a second type of neutron spectrometers: direct time-of-flight (TOF) spectrometer, with very large pixelated detector banks that have become the second standard instrument for single crystal neutron spectroscopy. They allow mapping large volumes of  $(q, \omega)$  space, but require short incoming pulses which provide a low intensity of neutrons onto the sample. They therefore require large samples (up to 100g co-aligned single crystals) and hours to days of counting per setting, which is not suitable for parametric studies as function of temperature, magnetic field, pressure etc. They become particularly disadvantageous in combination with large split-coil magnets or large pressure cells (anvil type), which only offer a narrow horizontal plane of scattering, hence only illuminating a fraction of the detector bank.

An alternative approach to direct geometry ToF spectrometers is indirect geometry ToF spectrometers. Indirect ToF use crystal analysers to determine the final energy of neutron after scattering, like an analyser on a TAS. By recording the total flight path time and the

detector into which the neutron is scattered the wavevector and energy of the neutron can be determined. Whereas a direct ToF uses a fraction of the neutron incident beam using a monochromating chopper, an indirect ToF can use a broad bandwidth polychromatic neutron incident beam to have a very large flux advantage over direct ToF. A direct ToF makes up for the low incident flux by detecting as large a possible solid angle of scattered neutrons of all final neutron energies, whereas present indirect instruments detect only one final energy of neutrons for neutrons scattering near the horizontal plane.

At the ISIS facility the indirect ToF instrument PRISMA was the first spectrometer at ISIS to study the wavevector dependence of excitations in single crystals. The PRISMA concept underwent different development processes, identifying the difficulties of this type of instrument and the developments required to advance indirect ToF instrumentation. ISIS currently has two indirect ToF spectrometers in user operation working in backscattering geometry to achieve very high energy resolution, the ultra-high resolution Iris, and the high resolution Osiris instruments. Osiris has proven to be a very powerful spectrometer for studying magnetic excitations in single crystals[2].

To fill the gap between traditional TAS instruments and TOF instruments, novel instrument designs have evolved. These designs started with the RITA concept (Re-Invented Triple Axis spectrometer), which employed a large modular multi-analyser system compared to a single analyser of a traditional TAS[3]. Proposers in this work unit were active in the commissioning of the original RITA spectrometer at Risoe National Laboratory in Denmark, and in the design and commissioning of the RITA-2 spectrometer at PSI. A multi-analyser system works by recording neutron scattering simultaneously at a different wavevector for each analyser, unlike the point by point measurement of excitations by a traditional TAS. Several other multi-analyser TAS instruments covering an even larger number of angles with more analyser channels have been developed, and are in regular user operation[4-6]. The new multi-analyser TAS instruments measure typically 30 channels, but with each channel having less intensity than standard double focusing TAS analyser, with the analyser channels typically covering only 30-40° of scattering angle. This can be achieved by having 30 analysers arranged in a fan around the sample position, scattering the neutrons either in a horizontal sense like the MAD concept at the ILL, or scattering neutrons vertically like the Flatcone concept at the ILL. Scattering neutrons vertically has the advantage of being able to place the neutron detectors in a well shielded position, drastically reducing background neutrons scattering in to the detectors. The horizontal geometry can however use a double bounce analyser system to allow for the direct line of sight between the neutron detectors and the sample position to be heavily shielded from background neutrons, like the present version of the MACS spectrometer at NIST.

## **1c) CAMEA Instrument Concept**

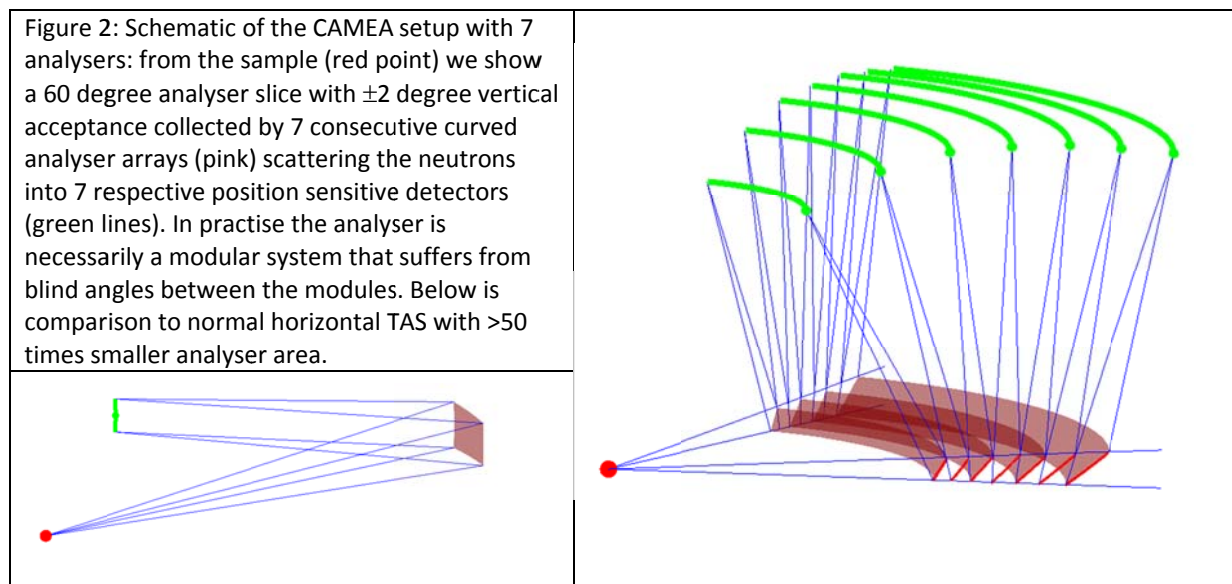
In a traditional TAS the back-end is a single analyser (flat or curved) that collects neutrons scattered into a certain solid angle element and with a certain final energy. The sample however scatters neutrons in many different directions and energies. Hence, tremendous gains in data collection rates can be achieved by collecting scattered neutrons over a larger solid angle and with differing energies. Direct geometry time-of-flight instruments detect neutrons scattered from sample over as wide a possible solid angle to increase neutron detection efficiency, but to be able to resolve the energy of neutron short pulses of



monochromatic neutrons must be cut from the incident neutron beam. Thus direct geometry spectrometers use only a small fraction of the available neutrons. To this end, we have developed the novel CAMEA indirect geometry spectrometer concept.

The novelty of the proposed CAMEA (Continuous Angle Multiple Energy Analysis) spectrometer is that it employs a series of 10 analyser arcs placed behind each other, where neutrons are scattered vertically into position sensitive detectors. The position the neutron is detected in the detectors determines the scattering angle of the neutron, while the analyser crystal determines the energy of the scattered neutron, which is combined with the time of flight to determine the energy transferred to the sample. Neutrons that are scattered to a different final energy by the sample will not fulfil the scattering condition at the first analyser, and hence continue straight through it. By placing subsequent analyser arcs, several different final energies of the scattered neutron can be measured simultaneously. Working as an indirect geometry time of flight instrument means that each analyser arc of CAMEA sweeps an energy range of excitations in the horizontal scattering plane, with different energy resolutions for each arc. The CAMEA concept arguably realises the most efficient in-plane spectrometer possible.

Transmission through the Pyrolytic Graphite analyser crystals is 98.5 % per mm - sufficiently high that more than 10 crystals of 1 mm thickness can be used, but the increasing analyser radius and increasing vertical size of the analyser renders arrays beyond 10 increasingly expensive for crystal material. We therefore aim for 10 analyser arcs, designed in a modular fashion. Prototype testing of CAMEA will enable calculation of the optimum number of analyser arrays to achieve maximum counting efficiency. Likewise, the spectrometer will employ analyser segments to cover as large as possible angular range that shielding of the neutron beam guide allows, potentially  $\pm 150^\circ$ .



CAMEA can be thought of as an evolution of the Prisma concept at ISIS. Prisma-II used one set of analysers with the scattered neutrons analysed at one energy for each scattering angle

covered, with analysers scattering the neutrons horizontally. With detectors in the horizontal scattering plane and little neutron absorbing material between the detectors and the sample position, PRISMA-II suffered from a high background count. The next generation PRISMA-III used a double bounce set of analysers to analyse the scattered neutrons energy, this allowed for heavy neutron shielding to be placed in the direct line of sight between the sample position and the detectors. The double bounce analyser system restricts the angular coverage, so although PRISMA-III had a good background, the large number of steps required to create a scan made this version of PRISMA inefficient. PRISMA-III is similar to the MACS multiplexed TAS concept developed and in user operation at NIST[4]. A new generation PRISMA-IV was envisaged to increase counting efficiency, in which a single set of analysers scatter the neutrons vertically into detectors. This geometry allows for heavy neutron shielding to be placed in between the sample position and detectors, without restricting the analyser coverage. The PRISMA-IV geometry has been realized and is in user operation in the Flatcone multiplexed TAS option at the ILL. CAMEA takes the PRISMA-IV concept an evolutionary step forward by using many analyser sets that simultaneously record excitations of differing energy ranges, with different energy resolutions, achieving a far higher efficiency of neutron detection in the horizontal scattering plane.

CAMEA removes additional shortcomings from which PRISMA suffered. PRISMA had a wider bandwidth of neutrons falling on the sample position than required, so that a neutron Laue diffractometer could be placed after PRISMA. The extra bandwidth of neutrons falling on the sample position of PRISMA increased the background counts. Computing capabilities to run PRISMA were limited, but advances in computing power have removed this problem. The success PRISMA experiments, like that of TAS experiments, relies on choosing the correct instrument resolution setup, whereas the CAMEA concept allows for excitations at the same energy to be simultaneously measured by different analyser arrays with differing energy resolution. CAMEA will also take into account the experience of instrument responsables working with the Flatcone option at the ILL, that have shown the importance of using radial collimation on spectrometers to remove the visibility of the sample environment for the secondary spectrometer.

## 1d) Instrument Parameters

In the following table we outline the starting parameters envisioned for the CAMEA spectrometer that are to be optimized during instrument development:

Parameter	Specification
<b>Moderator</b>	Cold
<b>Pulse shaping chopper to sample distance</b>	165 m
<b>Guide System</b>	Feeder into virtual source, followed by double elliptical guide with kink between ellipses to remove line-of-sight to the source.
<b>Neutron incident wavelength</b>	1-8 Å
<b>Flux at sample position[8]</b>	$1.8 \times 10^{10}$ neutrons per second per cm <sup>2</sup>
<b>Maximum Sample Size For Optimal Resolution</b>	5 mm by 5 mm
<b>Effective beam size at sample position</b>	15 mm by 15 mm
<b>Maximum beam divergence at Sample Position</b>	$\pm 2^\circ$ vertical $\pm 1.5^\circ$ horizontal
<b>Q- range</b>	0.04-7.1 Å <sup>-1</sup>
<b>Final energies of PG002 analysers[9]</b>	2.5, 2.8, 3.1, 3.5, 4, 4.5, 5, 5.5, 6.5, 8 meV
<b>Fixed or variable final energies?</b>	Fixed final energies
<b>Angular coverage of Scattered neutrons</b>	$3^\circ < 2\theta < 135^\circ$ for every analyser energy
<b>Sample to Detector distance</b>	1.8 to 3.25 m
<b>Neutron Detectors</b>	2.4 m <sup>2</sup> - <sup>3</sup> He or solid state detectors

The CAMEA instrument achieves significant gains from:

- 1) Using a medium bandwidth white neutron beam increases flux by more than an order of magnitude over the maximum triple axis spectrometer flux at high flux reactors. Optimized use of ESS long pulse will give a gain factor of over 200 compared to the flux of indirect geometry spectrometer Osiris at the ISIS facility[10]. And a flux advantage of more than 10000 over the direct time of flight chopper spectrometer IN5[11].
- 2) Increased efficiency in beam delivery using focusing neutron guides over using a crystal monochromator.
- 3) A fourfold or greater increased angular coverage of scattered neutrons for a single analyser array in comparison to the Flatcone and MACS multiplexed triple axis instrument concepts, or the PRISMA-III indirect geometry time of flight concept.
- 4) Advantages of a multi-analyser system

As CAMEA is being designed as a spectrometer that enables studies of small samples, we will investigate options such as the beam defining slit package of WISH to reduce the number of neutrons that reach the sample position but miss the sample, and cause an increase in the background[12]. Preliminary simulations indicate that instrument optimization for smaller beam size at the sample position does not increase flux density, but reduces the halo size of neutron beam at the sample position.

## 1e) Advantages of Multi-analyser System

Each analyser of CAMEA scans a specific wavevector and energy range. The analyser set to the smallest final neutron energy has the best resolution but covers the smallest region of reciprocal space, with the inverse being true for the analyser which reflect neutrons with the largest final energy. In this way data from different analyser arrays can provide a zoom for excitations measured at the same energy transfer.

For one measurement setup of CAMEA the analyser with the highest final neutron energy, will be measuring the excitations at the lowest energy transfers with the lowest energy resolution, the opposite to desirable situation. The converse is true for the analyser looking at neutrons with the lowest final neutron energy transfer, again opposite to the most desirable setup. In the general case not every analyser will provide equally important information. If, however, the experiment needs to determine accurately the dispersion at the zone boundary, for determining the strengths of weaker yet vitally important interactions, the scattering by different analysers of CAMEA matches the experimental needs.

The correct choice of energy resolution for an inelastic neutron scattering experiment can be vital for the success of an experiment. Estimates of the required resolution for an experiment can be wrong. If an experiment was being performed on a TAS with too low energy resolution, the measurements would have to be started from the beginning with a higher energy resolution. For CAMEA the instrument will be setup to perform an experiment with a specific energy resolution using a specific analyser, but the neighbouring analysers will be measuring excitations over similar overlapping energy ranges. Therefore, if the required resolution for the experiment is different to what was estimated, CAMEA will still be measuring excitations with the required resolution with a different analyser. This greatly reduces the potential of wasted neutron beamtime.

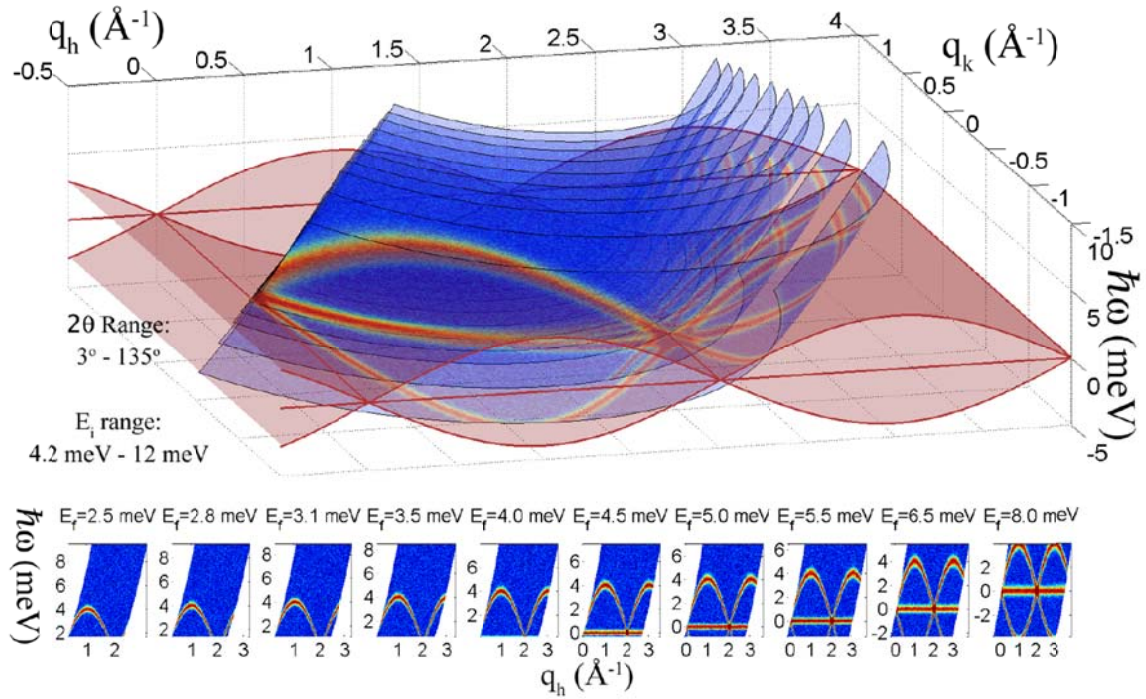


Figure 3: A diagram to represent the measuring capabilities of CAMEA measuring the magnon spin excitation spectrum of a one dimensional spin system, in one point scan. The main figure shows the surfaces in reciprocal space mapped by CAMEA, and the red surface represents the magnon dispersion. Below the main figure shows the projected excitation spectrum measured by the ten different analysers of CAMEA. No spinon continuum excitation is included, and dead angles between the analyser sections have been omitted.

As excitations will be measured at a specific wavevector and energy with differing energy resolution, simultaneous fits of the different data sets will increase the accuracy of mapping excitations in materials. Improvements in data fitting software will be required to maximise this potential.

In inelastic neutron scattering neutrons can scatter in an undesirable way from materials other than the sample in the neutron beam, or from multiple scattering events, and if these neutrons are detected they produce spurious additional counts. Techniques such as shielding, collimation, and filtering the neutron beam can reduce the number of spurious scattering events but not eliminate all spurious scattering. On CAMEA the same point in reciprocal space is measured with several analysers, so any remaining spurious scattering can readily be identified by comparison of data sets from different analysers and removed from the data.

A further advantage of the multi-analyser will be discussed in respect to CAMEA's capabilities in time resolved studies.

## 1f) Polarization analysis

Neutron polarization is a powerful tool in inelastic neutron scattering that user communities have requested as a day one priority for ESS instruments, see for example:

[https://maiserxx.esss.lu.se/press/GetInvolved/SymposiaReports/ESS\\_report\\_Boothroyd.pdf](https://maiserxx.esss.lu.se/press/GetInvolved/SymposiaReports/ESS_report_Boothroyd.pdf)

Hence, an option for polarization analysis on CAMEA must be considered. The D7 spectrometer at ILL is a working example of how polarization analysis can be successfully performed over a wide scattering angle in the horizontal scattering plane[13]. At present there are three proven techniques for producing polarized neutron and performing polarization analysis;- Heusler crystals, polarizing supermirrors, and He-3 spin cells. Here we outline the pros and cons of each polarizing technique for CAMEA. Our criteria for selection are as follows:

- 1) Wide angle analysis covering as large as possible scattering angle
- 2) Compatibility with extreme sample environments
- 3) Optimized for cold neutron spectroscopy
- 4) Ease of use, that requires rapid change setup from unpolarized to polarized neutron scattering

**Incident polarization:** Heusler crystals can only provide monochromatic neutron beams, which is not compatible with the CAMEA concept. Both He-3 spin cells and polarizing mirrors can be used to polarize the incident neutron beam over a bandwidth, and be an installed option using a guide changing section in the primary spectrometer. Ideally the incident polarizing option should be implemented without the need to access the neutron guide. The need to change He-3 cells during an experiment, or performing continuous re-filling of the He-3 spin cell, makes polarizing neutron supermirrors the preferable option. He-3 spin cells can however be used to polarize thermal neutrons, whereas supermirrors performance is poor for thermal neutrons.

Due to the time stability of a supermirror polarizer, we choose this option to produce polarized neutrons for CAMEA.

**Polarization analysis:** All three options for polarization analysis of the outgoing neutron beam can be used. Heusler analyzers are a proven technique but the reflectivity of heusler is significantly lower than Pyrolytic graphite or Si, and the required magnetic yoke would prohibit the possibility of using analyzers placed behind each other. A magnetic yoke greatly reduces the transmission of neutrons, and the yoke requires a large volume of space, so it is not possible to place Heusler analyzers with magnetic yokes behind each other. A wide angled He-3 spin cell could be used to analyse the scattered neutrons, the ISIS facility, ILL and Juelich have all been developing this concept which is commonly known as PASTIS. There are at least two large problems for using a PASTIS option on CAMEA. The sample space diameter of PASTIS options is typically ~6 cm, and this would need to be dramatically enlarged to be compatible with extreme sample environments, e.g. a 60 cm diameter cryomagnet, with the cost of He-3 cell approximately increasing with the cube of their diameter. Secondly the He-3 cell depolarizes in the presence of magnetic fields, therefore stray fields from cryomagnets would be a problem. This leaves a polarizing supermirror bender to analyse the scattered neutron polarization, which is a proven technique on D7 at

the ILL, and is compatible with using a series of analyser arrays placed afterwards. Stray magnetic fields from cryomagnets cause two problems that need to be addressed, induced stress on a supermirror bender, and the ability of neutron spin flippers to function.

The cost of supermirror polarization analyzer for CAMEA is of the order of 3 million Euros, estimation provided by Thomas Krist (HZB, Neutron Optics Berlin).

## **2) Experimenting Capabilities of CAMEA**

### **2a) Measurement Techniques**

#### **2a.i) Mapping**

The biggest break-through in inelastic neutron scattering of the last decade has been brought about by spectrometer innovations that enable full mapping of the reciprocal space, in wavevector and energy. After the success of using position sensitive detectors bank on HET, the MAPS spectrometer at ISIS was conceived as a direct geometry time of flight instrument utilizing 100% position sensitive detectors. MAPS lead directly to break throughs such as the observation of the universal hourglass excitation spectrum of cuprate superconductors[14], and to the planning of many new direct geometry time of flight spectrometers around the world. In comparison to this, the traditional work horse of inelastic neutron scattering the triple Axis Spectrometer (TAS,) has been advanced by multiplexing options such as Flatcone. Multiplexed TAS allows for fast mapping of a single scattering plane one energy at a time.

CAMEA provides a method for measuring the excitations of a single scattering plane in a manner similar to Flatcone; by performing a crystal rotation scan. Using Time of flight analysis means that CAMEA records the excitations over a range of energies similar to a direct ToF geometry spectrometer, or to a scan of  $k_i$  on a TAS. Compared to a multiplexed spectrometer, CAMEA mapping simultaneously different energies equates to an order of magnitude gain in measuring simultaneously excitations for each analyser array. Whereas CAMEA gains with respect to direct geometry ToF instruments by increasing the magnitude of the incoming flux by a factor of the order of 100-1000. The flux advantage of CAMEA over a direct ToF will enable CAMEA to map excitations in the horizontal scattering plan faster, but at the cost of not examining the out of plane neutron scattering recorded on a direct ToF. But with extreme sample environments that restrict coverage to the horizontal scattering plane, only inplane excitations can be measured anyway.

Mechanical issues, and the need for neutron shielding for the secondary spectrometer of CAMEA, results in blind spots in the angular coverage. A complete mapping of excitations by CAMEA in one sample rotation scan can be achieved by examining data taken by the different analyser arcs.

## **2a.ii) Parametric Studies by Single Acquisition Scans**

In inelastic neutron scattering important information can be obtained by determining the development of excitations at specific  $(q, \omega)$  points in reciprocal space with respect to an external parameter, i.e. an applied magnetic field, temperature etc.. It is therefore important to measure such excitations repeatedly at different values of the external control parameter. In this way we study the development of features such as resonances, gaps and crossings of excitation branches. The ability of TAS to focus on a specific energy and wavevector have made TAS the instrument of choice for performing parametric studies by measuring point by point scans. CAMEA can perform scans for parametric studies in a more efficient way than TAS, the quasi-continuous coverage of CAMEA in the horizontal plane allows multiple wavevectors along an arc in reciprocal space to be collected simultaneously, measuring the excitation over a limited energy range. In this way CAMEA can measure a specific excitation in a single spectrometer position or point, and this excitation can be studied parametrically without the need to move the spectrometer.

## **2b) Measurement Possibilities with CAMEA**

### **2b.i) Time Resolved Studies**

Inelastic neutron scattering studies the dynamics of the equilibrium states of materials, to fully understand materials we need to determine how systems that are pushed out of equilibrium relax back to their equilibrium state. Our present microscopic understanding of interactions of the out of equilibrium states is based mainly on our knowledge of the equilibrium state. An example of out of equilibrium studies that can presently be performed are studies using the pump probe technique. The experimental possibilities for the uses of neutron scattering in time resolved studies have been identified[15], yet the use of time resolved studies is limited by current instrument capabilities. The ESS provides an opportunity for inelastic neutron scattering to study out of equilibrium dynamics that potentially will lead to break through understandings and discoveries of the properties of materials. We envisage that such experiments will be limited by low neutron count rates, concentrating on focused studies of specific  $(q, \omega)$  excitations in reciprocal space.

The CAMEA concept provides a powerful measuring tool for out of equilibrium studies, because of the instrument's good time resolution. For CAMEA the time uncertainty for when a neutron was in the sample is governed by the uncertainty in the flightpath of the neutron from scattering in the sample to its detection. The energy of the scattered neutron is determined by the crystal analysers. Estimates for the flight path uncertainty have been calculated to be  $\sim 20 \mu\text{s}$  for every analyser arc, with the focusing geometry being the main source of uncertainty. An excitation at a specific energy can be studied at the same energy transfer for approximately 2.86 ms, the timewidth of the ESS source pulse, with a  $\sim 20 \mu\text{s}$  time resolution. Furthermore each analyser arc will be looking at an excitation at a different



energy transfer during this time. In this way single point acquisition scans can be used to study excitations in polycrystalline and single crystals.

CAMEA therefore can provide the time dependence simultaneously of single acquisition scans from each analyser at a different energy, in one data collection setup. The CAMEA secondary spectrometer can be installed on a triple axis spectrometer at a continuous flux neutron source, but with the requirement to move around a monochromator the angular coverage would be restricted to one quarter of that possible for CAMEA at the ESS. For time resolved studies the peak flux is the important factor, which is a factor  $>10$  larger at the ESS than for a continuous source. At a continuous source, however, there is no time limit to how long an excitation can be studied in time resolved studies.

Having identified the potential for time resolved studies with the CAMEA spectrometer it is important to identify what this ability can be used for. Magnetic fields can be used to tune the states of magnetic materials as will be discussed in section 3a). At present the number of systems and transitions that can be studied are limited by the maximum achievable steady state magnetic field in neutron scattering. Very recently in experiments performed at the ILL have shown that easily high magnetic fields of 30 T pulsed fields can be achieved to examine cyclic transitions with neutron scattering. The Full Width Half Maximum of the such a pulsed field is  $\sim 2\text{ms}$  [16]. There is on-going work to increase the duty cycle of the magnets and hence counting time. It is also possible to increase the maximum magnetic field at the cost of the pulse width. Working with pulsed magnets the time resolution of CAMEA allows for highly accurate determination of the fields of transitions, to resolve the time/field evolution of both the ordering and decay of the field induced states, and the ability to resolve the highest magnetic fields from shorter pulse widths.

For a direct geometry TOF spectrometer the energy of the neutron and the time uncertainty of when that neutron was in the sample are determined from the time uncertainty of the neutron flight path from the monochromating chopper to neutron detection. That is, at each pulse one position in reciprocal space over one time interval will be measured. A 3 ms time decay of a specific location in reciprocal space with  $40\text{ }\mu\text{s}$  time resolution would therefore take 75 scans. These 75 scans would however be mapping the excitations over other energies and wavevectors, containing potentially useful data.

Out of equilibrium time resolved studies require sample environments a level of complication greater than the simplest neutron sample environment, to push systems out of equilibrium. We have already highlighted the advantage CAMEA has in performing experiments with such sample environments, due to background reduction by radial collimation and the high incident neutron flux used by CAMEA.

## 2b.ii) Small Samples Studies

A present limitation of inelastic neutron scattering is the need for large samples to perform experiments on, typically  $1\text{ cm}^3$  in size. This limits inelastic neutron scattering to only materials that can have large samples grown, effecting:

i) Many materials cannot be grown in large volumes, due to stresses and strains in their structure. For example magnetic materials with high degrees of spin frustration are systems that are typically cannot be grown as large crystals. This limits studies of material classes and phenomena to a small number of materials that can be grown. The fact that only certain materials can be grown into large samples is suggestive that these materials are non-typical. In the case of copper based high temperature superconductors research with inelastic neutron scattering has been restricted mainly to La and Y based materials, leading to a fierce debate on the magnetic interactions of high temperature superconductivity in copper based materials[17]. By enabling inelastic neutron scattering to be performed on smaller crystals the number of materials available for experimentation drastically increases, allowing for identification of global behaviour over material specific properties.

ii) When new materials are discovered, inelastic neutron scattering has to wait a significant time until large samples can be grown to perform experiments. This limits the impact of inelastic neutron scattering, but more importantly allows for incorrect over interpretation of results from other techniques, on issues that inelastic neutron scattering can resolve. The lack of input from inelastic neutron scattering may lead to misdirection of experimental and theoretical studies of these materials.

iii) Neutron absorption by the sample material results in an optimum sample size, where increasing the sample size to increase neutron scattering rate is negated by neutron absorption. For samples with high neutron absorption, this size may be of the order of mm's. Here, the only improvement in inelastic scattering data therefore comes from instrument development.

iv) The crystalline quality of materials can bring into question whether the measured excitations display intrinsic or extrinsic characteristics of materials. Large  $1\text{ cm}^3$  sized crystals have a mosaic quality, a variation of composition, and are normally far from being perfect crystals. In general a small single crystal can be produced to a higher quality than a large single crystal of the same material. The higher quality crystals allow for the studying intrinsic behaviour closer to the ideal physical behaviour.

v) Extreme sample conditions can be used to manipulate the properties of materials into desirable phases, and across phase transitions. The greater extremes required, the smaller the sample volume becomes due to energy and mechanical restrictions, whereas the scientific possibilities increase with increasing extremes. To maximize the use of inelastic neutron scattering under extreme conditions requires an instrument optimized for small samples.

The optimization of CAMEA flux is for maximum intensity for 15 mm by 15 mm neutron beam cross-section at the sample position, with a neutron halo of double this size in both directions. A small beam size at the sample position will be achieved by the ability to tightly define the incident neutron beam with a series of jaws to reduce the number of neutrons not

reaching the sample position, this concept has been implemented on the WISH instrument at ISIS [19]. The beam definition jaws can define the beam size at the sample position and the vbeam divergence, thus reducing the halo of neutrons of background scattering from neutrons not hitting the sample position.

## **2b.iii) Rapid Identification**

From material's structure and their bulk properties, materials are identified as being close to or an actual realization of theoretically predicted phases of matter. For magnetic systems inelastic neutron scattering provides a definite way to determine if the systems are model candidates for different magnetic states. Quick mapping of the excitation spectrum on CAMEA could be used as a way to systematically identify if materials are realizations of model spin systems. For example the recent observation of an hourglass excitation spectrum in an iron based superconductor suggests that new classes of high temperature superconductors could be searched for by identifying materials in which hourglass magnetic excitation spectra occur[20]. Rapid mapping could readily be open to users in an express operation mode, such as Merlin EXPRESS at ISIS, enabling users to gain neutron beamtime in the short term.

## **2b.iv) In-situ Studies**

A great advantage of direct geometry ToF spectrometers is the clean excitation spectra that can be measured when the amount of material in the neutron beam is kept to a minimum, such as a closed cycle refrigerator. Extreme sample environment however place lots of support material in the neutron beam, from which neutrons scatter off to produce structured background detector counts. The visibility of sample environment can be dramatically reduced by using collimators. This is a standard practise for performing neutron diffraction in extreme environments, but is not presently standard practise when using spectrometers due to the vast number of experimental configurations used on spectrometers. Spherical radial collimation required for a direct geometry time of flight spectrometer is hard to envisage in a flexible way for an instrument that is a general purpose spectrometer. As an instrument designed for extreme environments CAMEA can and will include radial collimation to reduce visibility of sample environment. Extreme sample environments are not the only sample environments that place large quantities of material in the beam, the same is true for in-situ studies of materials inside working components or reaction cells. CAMEA will therefore provide a clean way of performing measurement of excitations in in-situ experiments. The scientific drivers for in-situ experimentation for different field of research have been discussed in the ESS Technical Design Report, Chapter 2 Neutron Science.

## **2b.v) Actinide Heavy fermion Systems**

Heavy fermion systems remain a major area of research in magnetism that has been under investigation for decades. The underlying physics of magnetic materials from the 4f and 5f elements is dramatically different to that of the transition metals in part due to the differing extent and orbital character of the systems electrons. Neutron scattering is an ideal probe of the magnetic interactions of these materials, but in many for many actinide elements neutron absorption activates the system leading to a decay that produces neutrons. The neutrons produced by the activated sample lead directly to background detector counts on direct geometry ToF instruments, rendering measurements of the excitation spectrums not possible. CAMEA shares two advantages with TAS that will enable it perform studies on the magnetic interactions of heavy fermion systems. 1) The neutron detectors have no direct line of sight view of the sample and significant neutron shielding is located between the sample and neutron detectors. 2) For any neutrons not absorbed by the shielding the solid angle of the detectors is small enough that the number of background neutrons that reach the detector is very low. These two points have been proven in a vast number of inelastic neutron scattering studies on heavy fermion systems using TAS.

## **2c) Extreme Conditions for Neutron Scattering**

### **2c.i) Existing Neutron Extreme Sample Conditions**

CAMEA is optimized for maximizing counting efficiency in the horizontal plane and to be compatible with extreme sample environments. An important question to answer is what we mean by extreme environments for performing inelastic neutron scattering. In this section we will identify what extreme sample environments are possible today that can be used on an instrument that is optimized for scattering in the horizontal plane.

In inelastic neutron scattering three extreme sample conditions are commonly employed for studying samples, namely temperature, magnetic field and pressure. It is often found that experiments require two extreme environments, typically low temperature combined with either high magnetic fields or high pressure. In the following table we list the extremes of sample environments that have been shown to be viable, or are in regular use, for inelastic neutron scattering.

Condition		Temperature Extreme (K)	Extreme Condition	Maximum Sample Size
Low Temperature	Dilution insert	50 mK		1 cm <sup>3</sup>
High temperature	Levitation furnace	3000 K		
Vertical High Magnetic field	Nb based Superconducting cryomagnet	1.5 K	16 T (symmetric)	2 cm <sup>3</sup>
	-With dilution fridge	50 mK	16 T	1 cm <sup>3</sup>
	-With 2.0 T permanent magnet boosters <sup>*</sup>	1.5 K	18 T <sup>*</sup>	133 mm <sup>3</sup>
Horizontal Magnetic field with horizontal access	Nb based Superconducting cryomagnet with 180° of dark angles	1.5 K	6.8 T	1 cm <sup>3</sup>
High Pressure	Paris-Edinburgh cell	300 K	130 kbar	~50 mm <sup>3</sup> single crystal
	Paris-Edinburgh cell	3 K	50 kbar	
	Paris-Edinburgh cell <sup>Δ</sup>	2000 K	70 kbar	

<sup>+</sup> Raffaele Gilardi<sup>1</sup> Journal of Neutron Research **16**, 93 (2008)

<sup>\*</sup> In practise the record is 17.9 T achieved in a nominal 15 T vertical cryomagnet at HZB, formerly HMI[21]. The 16 T maximum vertical field is a Bruker magnet named Fat Sam at ORNL.

<sup>Δ</sup> Y. L. Godec, M. T. Dove, S. A. T. Redfern, M. G. Tucker, W. G. Marshall, G. Syfosse and S. Klotz, High Press. Res. **23**, 281 (2003).

We conclude that a wish list for extreme environments for CAMEA that are achievable with present technology is as follows:

- 1) Vertical split coil superconducting magnet with the highest possible available field
- 2) A dilution insert with a base temperature of 50 mK
- 3) High pressure cells that perform as good as or better than the currently available Paris-Edinburgh cells, one for low temperatures (<300 mK), and one for high temperatures (> 2000K).
- 4) A wide bore vertical split coil superconducting magnet (>10T) for a pressure cell (>3 GPa) that can be cooled to <1K.

In the next sections of this report we will highlight the needs for these different experimental extremes, and highlight the science that CAMEA can do beyond the capabilities of present day instrumentation without further development of extreme sample environments.

## 2c.ii) Present Neutron User Community for CAMEA, and User Demand for an Extreme Environment Spectrometer

An indicator of the size of the present user community is the demand for beamtime on available instruments. CAMEA will be an instrument optimized for extreme sample environments, a cold indirect time of flight spectrometer, with an energy resolution a factor of 1.5-2 better than a cold triple axis spectrometer. With this optimization criteria for CAMEA we have obtained information on the user demand for instruments in Europe that study predominately magnetic excitations, that is cold triple axis spectrometers, and time of flight spectrometers. Direct geometry time of flight spectrometers such as IN5 at the ILL. are not included as a large proportion of their beamtime is used for soft matter, experiments that do not require extreme sample environments. As ultra-high energy resolution is not required for the experiments envisaged on CAMEA, we do not include information on high resolution backscattering instruments.

The overload demand for instruments was determined from the ratio of days requested for in beamtime proposals, compared to the number of days available to perform experiments on those instruments. This information was obtained from instrument responsables of each instrument. In the table below we record those figures. Each type of sample environment is listed separately in the table even though there is a significant overlap between demands for different sample environments, i.e. for low temperature measurements in an applied magnetic field.

Instrument (Neutron Source/institution)	Overload <sup>*</sup>	Magnetic fields (%)	Pressure (%)	1 K < (%)	Polarized Neutrons (%)	Furnace (%)
RITA-II, TASP (PSI)	2.5	33.9	4.3	19.2	N/a	
PANDA (FRM-II)	2.7	30	5	20	N/a	
LET (ISIS) <sup>#</sup>					Commissioning	
IN14 (ILL)	2.5	30-40	< 5	60	20-25	
IN12 (JCNS@ILL)	2.6	23.5	-	27.5	9.8	3.9
Osiris (ISIS) <sup>**</sup>	2	40		40	Planned	
FLEX (HZB)	1.53	56.3		19.9	Commissioning	

<sup>\*</sup> The overload of an instrument is defined as the number of days applied for experiments divided by the total number of days available to perform experiments. <sup>#</sup> Requested <sup>\*\*</sup> The data for OSIRIS is for before LET came into operation, stabilization of proposal demand between the two instruments is yet to occur. <sup>+</sup> No information has been provided

**Table 1:** The demand for European based cold spectrometers that concentrate on magnetic excitations, and the demand for extreme environments conditions on these instruments.

The user demand for the present spectrometers is strong with over load factors between 2 and 2.7 for all instruments. This high demand for beamtime has resulted in a large investment in cold spectroscopy instrumentation. In the last seven years the number of spectrometers has been increased by the addition of LET, PANDA and the inelastic setup of

OSIRIS, as well as augmented by upgrades to FLEX and IN12. Upgrades are planned for IN14, RITA-II and an additional polarized cold triple axis spectrometer instrument is planned for the FRM-II reactor. The large user base of these instruments is a well-established community of inelastic neutron scatterers studying magnetic excitations, whom are skilled at performing experiments, and performing detailed data analysis.

For the instruments of table 1 the demand for extreme conditions approximates to 40% of proposed experiments. With no dedicated extreme environment spectrometer existing, this represents a substantial demand for beamtime, especially when we consider that all systems studied under extreme conditions are first studied under nominal conditions. The beamtime demand for inelastic neutron scattering to study materials under extreme conditions shows that there exists a strong user base within the present user community of cold spectrometers in Europe. In the September 2011 ESS science symposium on Strongly Correlated Electron Systems, neutron users from this user community who study magnetic excitations stated that an extreme conditions spectrometer was one of their top three neutron instrument desires for the ESS.

We note that present demand for cold inelastic neutron spectrometers using a high pressure sample environment is low. We will highlight in examples of the science CAMEA will enable, and we will explain why pressure is low demand for inelastic neutron scattering. The main reason pressure cells are not regularly used is that the maximum samples dimensions that can be used with pressure cells is too limiting for feasible inelastic neutron scattering experiments with present neutron instrumentation.

CAMEA as an instrument that is optimized for inelastic neutron scattering in extreme environments the output of experiments in extreme environments on CAMEA will be higher than for a general instrument. In this way CAMEA would act as an ideal complement to a general purpose cold chopper spectrometer.

Demand for extreme spectrometer from ESS symposium:

[http://europeanspallationsource.se/sites/default/files/spin\\_dynamics\\_of\\_correlated\\_electron\\_systems\\_2012.pdf](http://europeanspallationsource.se/sites/default/files/spin_dynamics_of_correlated_electron_systems_2012.pdf)

Recent Publication highlights of inelastic neutron scattering performed under extreme conditions at neutron facilities in Europe:

Quantum Criticality in an Ising Chain: Experimental Evidence for Emergent  $E_8$  Symmetry. R Coldea, D. A. Tennant, E. M. Wheeler, E. Wawrzynska, D. Prabhakaran, M. T. F. Telling, K. Habicht, P. Smeibidl, and K. Kiefer, *Science* **327** 177-180 (2010).

Spin fluctuations in normal state CeCu<sub>2</sub>Si<sub>2</sub> on approaching the quantum critical point. Arndt J., O. Stockert, K. Schmalzl, E. Faulhaber, H. Jeevan, C. Geibel, W. Schmidt, M. Loewenhaupt, F. Steglich, *Phys. Rev. Lett.* **106**, 246401-1-246401-4 (2011)

Magnetically driven superconductivity in CeCu<sub>2</sub>Si<sub>2</sub>. O. Stockert, J. Arndt, E. Faulhaber, C. Geibel, H. Jeevan, S. Kirchner, M. Loewenhaupt, K. Schmalzl, W. Schmidt, Q. Si, F. Steglich, *Nature Phys.* **7**, 119-124 (2011)

Resonant magnetic exciton mode in the heavy-fermion antiferromagnet CeB<sub>6</sub>. G. Friemel, Y. Li, A. V. Dukhnenko, N. Y. Shitsevalova, N. E. Sluchanko, A. Ivanov, V. B. Filipov, B. Keimer, D. S. Inosov, *Nature Communications* **3**, 830 (2012).

Mixed acoustic phonons and phase modes in an aperiodic composite crystal. B. Toudic, R. Lefort, C. Ecolive, L. Guérin, R. Currat, P. Bourges, T. Breczewski, *Phys. Rev. Lett.* **107**, 205502 (2011).

Magnetic-field-induced soft-mode quantum phase transition in the high-temperature superconductor La<sub>1.855</sub>Sr<sub>0.145</sub>CuO<sub>4</sub>: An inelastic neutron-scattering study. J. Chang, N. B. Christensen, C. Niedermayer, K. Lefmann, H. M. Rønnow, D. F. McMorrow, A. Schneidewind, P. Link, A. Hiess, M. Boehm, R. Mottl, S. Pailhès, N. Momono, M. Oda, M. Ido, J. Mesot, *Phys. Rev. Lett.* **102**, 177006 (2009).

Magnetic-field-enhanced incommensurate magnetic order in the underdoped high-temperature superconductor YBa<sub>2</sub>Cu<sub>3</sub>O<sub>6.45</sub>. D. Haug, V. Hinkov, A. Suchaneck, D. S. Inosov, N. B. Christensen, C. Niedermayer, P. Bourge, Y. Sidis, J. T. Park, A. Ivanov, C. T. Lin, J. Mesot, B. Keimer, *Phys. Rev. Lett.* **103**, 017001 (2009).

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## **2c.iii) Future developments in Neutron Scattering for CAMEA**

### **Focusing Optics for ultra-small samples**

Neutron optics for focusing neutron beams down in size are continuing to be investigated at neutron scattering facilities such as the ILL and FRM-II. The neutron beam can be focused down by a focusing trumpet to gain neutron flux density at the cost of wavevector resolution and total neutron flux at the sample position. Providing CAMEA with an interchangeable end section to the neutron guide, will enable the installation of a neutron focusing device. This would provide the opportunity for CAMEA to study materials significantly smaller than the 5 by 5 mm beam size of the optimized instrument at the cost of significantly worsening wavevector resolution. Neutron focusing optics will be available to use before the start date of the ESS.

### **Cryomagnets**

The maximum obtainable magnetic field from a vertical split pair magnet can be advanced by the use of copper oxide based high temperature superconducting (cuprate) materials. Advancement of the highest available magnetic fields would open up research into many new materials that have been already identified at high magnetic field laboratories around the world. This research would investigate the complex phases transition and phenomena such as magnetic plateau states identified in high magnetic field laboratories that have not been resolved due to the lack of wavevector resolved studies that inelastic neutron scattering provides.

We note that a conceptual design study is being carried out by another ESS work package, with an estimated 25 T maximum field for a split pair magnet with horizontal neutron access[22]. The present cost of the cuprate superconducting tape required to make this magnet is however prohibitive. The magnet would only become affordable if improvements were made to production of the superconducting tape that leads to a reduction in the sale price. The timescale for improvements in production technique of cuprate material is hard to predict. The National High Magnetic Field Laboratory, USA, are developing 20+ T high temperature superconductor magnets, which will resolve the technical feasibility problems of construct such magnets[23].

### **Electric Fields**

The use of electric fields in neutron scattering is limited due to the size of electric fields in comparison to the typical neutron scattering sized sample. As the CAMEA concentrates on performing neutron scattering on smaller sized samples, studies of samples under applied electric field become increasingly feasible. We envisage that three dimensional control of the applied electric fields to investigate the single crystal polarization anisotropy to be desirable. Examples of present science that can be studied by applied magnetic fields are the manipulation of the magnetism of multiferroics, or the manipulation of skyrmion lattices.

## **Pressure Cells**

There is continuing effort to increase the capabilities of pressure cells for neutron scattering studies. In the following section we will outline the need to increase pressure cell performance for the geoscience community, and how this will be to the advantage for material science. There is a clear difference in capabilities between Paris Edinburgh cells used for neutron scattering experiments and the highest achievable pressures from diamond anvil cells at x-rays synchrotron sources[24]. The complimentary nature of the neutron and x-rays scattering technique ensure that the high pressure studies from x-ray experimentation will leave open questions in research. By increasing the available pressure range for neutron scattering, the high pressure user community of x-ray scatterers will have a new complementary experimental tool. One direction for advancing pressure cells will be discussed in the following geoscience section.

### **3) CAMEA for Science**

#### **3a) Magnetic Excitations in Applied Magnetic Fields**

Magnetic states of a material are the result of competition between different interactions occurring in materials. Materials that can be grown do not necessarily have the most desirable or intriguing magnetic interactions leading to a physically desirable state. In certain systems the magnetism can be changed by doping to change the magnetic state, but the doping process introduces structural impurities into materials, bringing into question whether intrinsic effects are being studied or extrinsic impurity effects. The use of magnetic fields offers an alternative approach to tuning magnetic interactions in a material. An approach in which the same sample and hence sample quality is kept, and the intrinsic magnetic interactions of materials are studied. Here we wish to briefly outline some of the phenomena that can be studied by inelastic neutron scattering under applied fields and what CAMEA will offer in neutron experimentation to these studies beyond current capabilities. In the following two examples we take two different cases of quantum magnets to discuss first detailed mapping of excitations and then discuss parametric scanning of excitation spectra. We are restricting our discussion in this section to what is achievable with CAMEA using the presently available cryomagnets.

The new magnetic states that are found by tuning the magnetic interactions under an applied magnetic field often contain many different excitation modes. Of these often the continuum excitation modes from deconfined excitations that are of greatest interest with the purest quantum character. Continuum excitation modes by their nature cover large areas of reciprocal space in wavevector and energy but are weak in intensity, requiring high intensity instruments to study them. Therefore studies of continuum excitations ideal require the flux of TAS but the mapping capabilities of a time of flight spectrometer, which CAMEA offers in combination. In figure 4 we highlight the state of art in theory and capabilities of the world leading cold TAS IN14. Theoretical calculations have dramatically advanced with computing power, so that calculations of excitation spectra surpass the capabilities of experimental studies. Measurements on IN14 were restricted in what could be determined to the magnetic state of the material and the observance of fractional spin excitations, but the results could not test the theoretical calculations. The capability of neutron instrumentation needs to be advanced to re-establish the positive feedback between theory and experiments to advance our understanding of novel quantum magnetism. CAMEA provides this advancement, and will provide for inelastic neutron scattering under applied magnetic fields an option comparable to high resolution neutron diffraction, studies of magnetic excitations in detail.

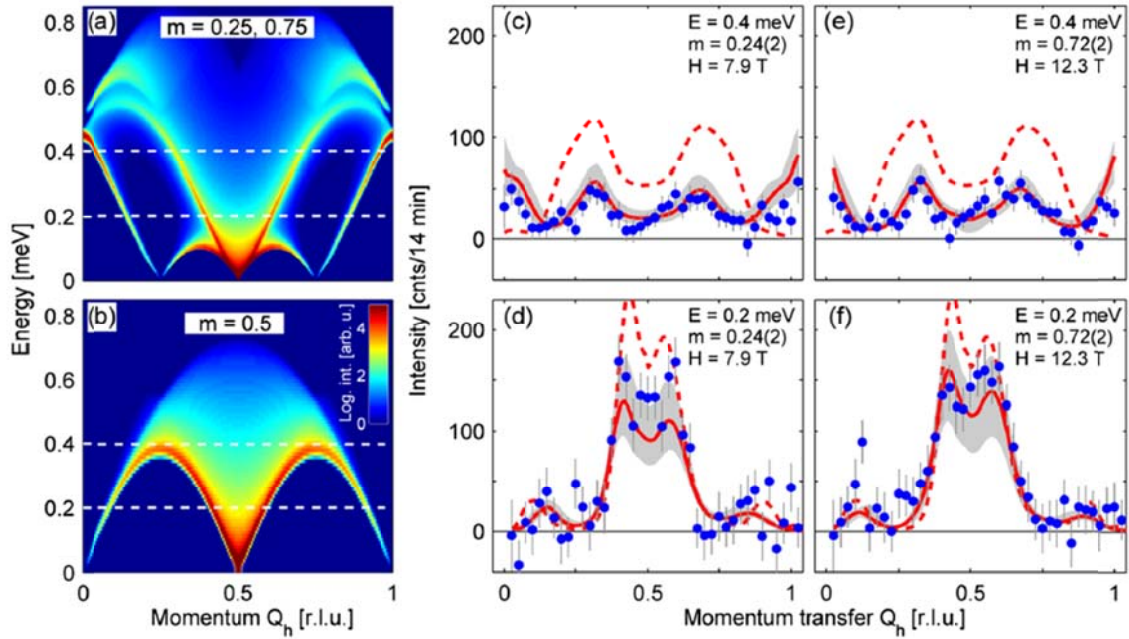


Figure 4: Inducing fractionalization of magnons in quantum spin ladder by application of a magnetic field. The spinon fractional spin excitations are observed as a weak excitation continuum between the sharp single magnon excitation modes. Left shows the theoretical calculation, and dashed lines indicated the scans that are shown in the centre and right panels on IN14. Theoretical calculations have surpassed the present measuring capabilities of inelastic neutron scattering. (Taken from Thielemann, Rüegg et. al. Phys. Rev. Lett. **102**, 107204 (2009).)

Quantum critical points (QCP) occur at a specific point in a phase diagram of certain materials, at this point quantum fluctuations dominate the material, and magnetic phase transitions are driven by quantum fluctuations. However a QCP has a very extended effect on the magnetic phase diagram. In figure 5 we show a typical QCP phase diagram, in  $\text{YbRh}_2\text{Si}_2$  the material is driven from an antiferromagnetic state into a Landau Fermi liquid phase at low temperatures. The colours of the phase diagram indicate two types of behaviour, normal Fermi liquid type behaviour in purple, and non-Fermi liquid type behaviour in orange, the later driven by the QCP. At present inelastic neutron scattering can elucidate magnetic excitations at specific energy and momentum transfers around QCPs, but measurements are very limited in tracking across the phase diagrams to scans at specific wavevectors or energies. The rapid mapping of CAMEA will change studies of critical phase transitions such as QCPs. CAMEA can collect rapid maps of the excitations spectrum where the structure of the excitation spectrum can be identified, and rapid maps can be collected repeatedly across the critical transition in a stepwise approach. In this way critical exponents can be identified, and the exact location in field of the QCP identified for detailed studies. From the critical exponents universality classes of QCP can be identified, and the basic theories of QCP tested. Rapid mapping can be thought of as providing the similar equivalence to low resolution parameter ramping experiments in neutron diffraction.

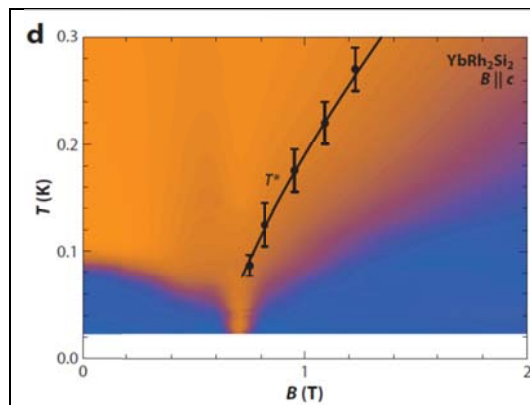


Figure 5: The magnetic phase diagram of  $\text{YbRh}_2\text{Si}_2$ , taken from J. Custers, *et. al.*, Nature 424, 524 (2003). With a quantum critical point occurring at  $\sim 0.75$  T at 0 K. The data points indicate Kondo breakdown as measured by resistivity. Purple indicates normal Fermi liquid type behaviour, whereas orange indicates non-Fermi liquid strongly correlated electronic behaviour

It is hard to predict what the future research into magnetism will be, but we would like to identify a couple of young fields of research that could prove to be as intriguing and rewarding as that of well-established phenomena such as high temperature superconductivity.

At present the research in magnetism is expanding beyond studies of materials based on transition metals from 3d row of the periodic table, to the 4d and 5d rows. For transition metals from the 4d and 5d elements of the periodic table the spin-orbit interaction strengthens from being quenched and near zero in the 3d transition metals. Theorists are studying the possibilities for new magnetic states within transition metal materials with spin-orbit interactions, and identifying theoretical possibilities of new phases of being, such as the quantum compass model[25]. The possibilities arising from the spin-orbit interaction for new magnetic states and studies of their potential use is a field of research in its infancy.

Research into 3d quantum magnets where electronic spin is a good quantum number are at an advanced stage for perfect model systems. The direction of research into the magnetism of 3d materials will therefore shift away from studying the perfect materials investigating the role of disorder, via impurity doping, bond disorder, and/or electronic doping. This research will be trying to identify protected states, phases of matter that are robust from disorder, surviving in imperfect materials, for example superconductivity is a protected state. Current interests in protected states revolve around topological materials, with a major recent finding being the discovery of magnetic monopoles in magnetic spin ices[26].

### 3b) Magnetic Excitations Under High Pressure

Pressure is an alternative tuning parameter of magnetic excitations, and pressure is distinctly differs from using applied magnetic fields. Pressure studies tune the magnetic interactions of the material by:

- 1) Altering bond angles, changing the magnetic path interactions and balance between different spin interactions in materials
- 2) Altering bond distances to alter spin interactions in materials
- 3) Pressure induced doping to study doping variation in a phase diagram

As applying pressure can simultaneously cause all of the above three effects, pressure can lead to tuning of the magnetic interactions in many different ways in phase space. Pressure can be used as a unique tool in this way to reach and go through phase transitions. In quantum magnetism, materials can be pushed through quantum critical points, and new quantum magnetic phases can be realized.

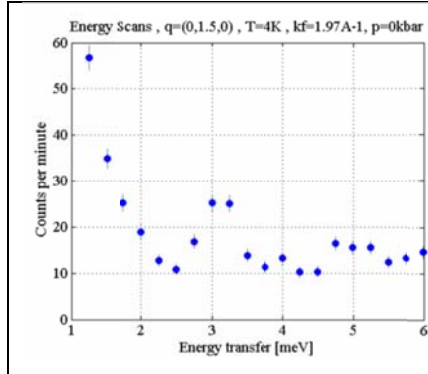


Figure 6: An energy scan of  $\text{SrCu}_2(\text{BO}_3)_2$  in a Paris-Edinburgh pressure cell on IN8 at the ILL. Below 2 meV the background rises due to background elastic scattering.

To reach the highest possible pressures we require the greatest possible force per unit volume. The maximum mechanical strength of pressure cells and the volume size of the sample are the two limiting factors of studying materials under high pressure. Paris-Edinburgh pressure cells have been proven an effective way to reach high pressures for

neutron diffraction, but the maximum volume for single crystals in a Paris-Edinburgh cell is  $\sim 50 \text{ mm}^3$ . It has been shown that magnetic excitations can be measured with a clean background in Paris-Edinburgh cells on the world's highest flux TAS, however the counting times prove to be prohibitive for performing inelastic neutron scattering studies. This limiting factor has restricted high pressure studies of excitations in inelastic neutron scattering to marginal use.

High pressure experiments on CAMEA would achieve two stages of advancement in spectroscopy under pressure. At present excitations at specific wavevectors can be studied under high pressure. The first advancement would enable determining the full dispersion of excitations along high symmetry directions, and the second stage would be that this is achieved by mapping the dispersion of excitations of an entire plane in reciprocal space. This advancement would enable phase diagram studies of excitations in materials under pressure that cannot be presently performed, revolutionizing the studies of excitations as direct geometry spectrometers with position sensitive detectors have previously advanced inelastic neutron scattering.

While this section has discussed high pressure studies with respect to magnetism, high pressure studies of phonon interactions are required to understand fundamental materials. As stated above pressure drives **changes** to the structure of materials, these structural changes alter the phonon modes of materials altering materials physical properties, and even lead to structural phase transitions, i.e. phases transitions driven by phonon softening. Phonon interactions under high pressure can be studied by inelastic x-ray scattering but the phonon excitation spectrum measured by x-rays is dominated by intensity of phonon modes arising from the heaviest elements. Therefore inelastic neutron scattering is needed to complement inelastic x-ray scattering, by determine the dispersion of phonon modes from light elements. For instance the different phases of water materials under high pressure continue to attract attention in high pressure neutron scattering[27]. With ability to perform phonon studies under extreme pressures and high temperatures having been already established [28].

### **3c) Strongly Correlated Electron Systems**

Strongly correlated electron systems are systems in which the properties of the materials are governed by collective behaviour of the electrons away from the limiting Fermi liquid behaviour of simple metals, and the single particle exchange interaction. Collective correlations result in novel phenomena such as charge order, orbital order, density waves, colossal magneto-resistance, multiferroicity, and superconductivity, to name a few active fields of research. Inelastic neutron scattering has played a crucial role in study the magnetic excitations in these materials, determining the magnetic interactions that participate in the collective behaviour.

In many strongly correlated electron systems the magnetic structure results in different spin domains, leading to differing magnetic structure. To resolve the many different excitation modes in strongly correlated systems it is desirable to have mono-domain samples, especially in the case of incommensurate magnetic structures. In certain materials the use of applied magnetic fields or applied pressure can create mono-domain samples. The classic example is using a magnetic field to create a mono-domain magnetic order in Cr; this enables studies of the many possible excitation modes, and lead to the beautifully complex yet incomplete theoretical description of Cr[29]. A complete understanding Cr still eludes, but remains a prominent question as the spin density wave state of Cr is often compared to the magnetic excitation spectrum of hole doped cuprate high temperature superconductors. Alternatively temperature, magnetic field or pressure can be used in as a perturbative interaction on strongly correlated electron systems.

Strong correlations often occur in materials with reduced dimensionality, in which the interactions are no longer three dimensional. In materials with reduced dimensionality, parametric studies need only to concentrate on the excitations in the scattering plane with the dominant interactions. As CAMEA is optimized to maximize the count rates from the horizontal plane, CAMEA is ideally suited for studies of excitation spectra in a specific scattering plane.

### **3d) Fundamental Understanding of Functional Strongly Correlated Electron Systems**

We have discussed ways in which CAMEA is suited to study strongly correlated electron systems, with a stress on understanding interactions in these materials. Several classes of strongly correlated electrons systems are of interest due to their physical properties, such as colossal magneto-resistance, multiferrocity, thermoelectrics and thermomagnetoeltrics materials. Colossal magneto-resistance and multiferrocity provide ways in which to manipulate magnetic memory, whereas thermoelectrics and thermomagnetoeltrics can be used in energy heat cycles. Inelastic neutron scattering provides a way to study the interactions of these materials to understand their fundamental behaviour, providing feedback into creating or discovering improved materials. CAMEA permits parametric mapping of the excitation spectra of these materials across their different phases, perform in-situ studies of these materials, and the possibility to study the time cycle of processes by time resolved studies not possible with present neutron instrumentation. Polarization

analysis on CAMEA enables the vital ability to disentangle magnon and phonon excitations, to understand the often important role of magnon-phonon coupling in these materials.

### 3e) Unconventional Superconductivity

Conventional superconductivity can be understood through the BCS theory of superconductivity, where phonon excitations mediate an attractive interaction between electrons enabling them to form Cooper pairs that can flow through materials without incurring an electrical resistance. Since the formulation of BSC theory there has been many discoveries of new classes of materials that superconduct but cannot be explained by BSC theory. These new classes of materials include heavy fermions, cuprates, cobaltates, ruthenates, pnictides, and chalcogenides. In these materials the formation of electron Cooper pairs and a superconducting condensate is not explained by BSC phonon mediation. Inelastic neutron scattering has provided a critical tool for identifying the magnetic origin of these new classes of superconductivity, discovering phenomena such as gapping of the magnetic excitation spectrum, and the occurrence of resonant spin excitations. While the origin and nature of these features in the magnetic excitation spectrums is unresolved, a magnetic origin for the superconductivity is commonly held belief.

Studies of unconventional superconductors typically require their excitation spectra to be studied at low energy transfers to study spin gaps, and resonance spin excitations, whereas to obtain the magnetic exchange interactions requires studies to large energy transfers. CAMEA will enable rapid mapping of the low energy excitation spectrum with high energy resolution. Rapid mapping can be used for identification of resonances, search for common characteristics of the magnetic excitations to identify unconventional superconductivity [16], and allow for parametric studies of the magnetic excitation spectrum evolution. An example of the limitations of present day inelastic neutron instrumentation is that it is still undetermined whether or not, resonance spin excitations in superconductors shift in energy with increasing temperature, and this is twenty years after the discovery in cuprates [30].

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### 3f) Soft Matter in Applied Magnetic Fields

The potential for use of applied magnetic fields has been examined as a potential research field for high magnetic field neutron scattering instruments[31], from which we will outline here.

Many studies of biological molecules benefit from techniques that aid in orienting the molecules. It has already been known for decades that molecules exhibiting anisotropic diamagnetism, can be aligned with use of high magnetic fields, provided the magnetic anisotropy and/or the size of the molecules is sufficiently large.

Nevertheless, magnetic orientation has not been used systematically in the past, but rather occasionally for particular types of materials, partly because often high magnetic fields are necessary. On the other hand, the application of a magnetic field has several advantages over other, more frequently used, alignment methods, since it leads to a bulk, contact free, non-destructive force, which is homogeneous throughout the sample and thus can be used for producing highly oriented bulk samples as well as thin films.

Magnetic fields are especially useful for orienting fibrous structures such as fibrin and for filamentous viruses and membranes. This magnetic field orientation is due to the diamagnetic anisotropy of the peptide and ester bonds. It is emphasized that structure determination is not the only goal of studies using magnetic orientation. For membranes, changes of protein binding at the membrane surface are important aspects of signal transduction and issues of amplification associated with specific events can be addressed, as has been done with the rhodopsin and transducin system of visual processes.

The change in diamagnetic energy depends on the size of the molecular aggregate. Therefore the higher the magnetic field, the smaller the molecular entity that can be aligned at room temperature. A larger the maximum available field increases the possibilities for alignment of liquid crystals and macromolecules at room temperature. At present research at steady state high magnetic fields laboratories such as that of Radboud University Nijmegen are taking advantage of the use of high magnetic fields for studying soft materials[32]. The studies being performed at high magnetic field laboratories show that potential for this technique increases with the maximum available steady state field, these fields are provided by extreme environment cryomagnets that can take full advantage of the CAMEA optimization.

### 3g) Geoscience

#### i) Scientific Motivation for Neutron Spectroscopy of Molecular Systems Under Extreme Conditions

Simple hydrogenated systems, like water, methane, ammonia, and their mixtures are systems of paramount importance for many fields in science, ranging from applied and environmental science to condensed matter and planetary physics[33]. These systems are widespread in the extra-terrestrial space, both interstellar and on outer planets, moons (ice bodies), and comets, and due to their relatively simple stoichiometry and electronic structure they represent key system for the study of molecular systems.

In the last few years, a tremendous effort has been invested by several groups around the world in the determination of the phase diagram of these systems up to very high pressures (-30 GPa), a program in which several European teams have been actively involved

With these data at hand, and with the information obtained from various spectacular space missions, the scientific community is currently trying to understand the interior of these bodies, the conditions of temperature and pressure, its chemistry (Figure 7).

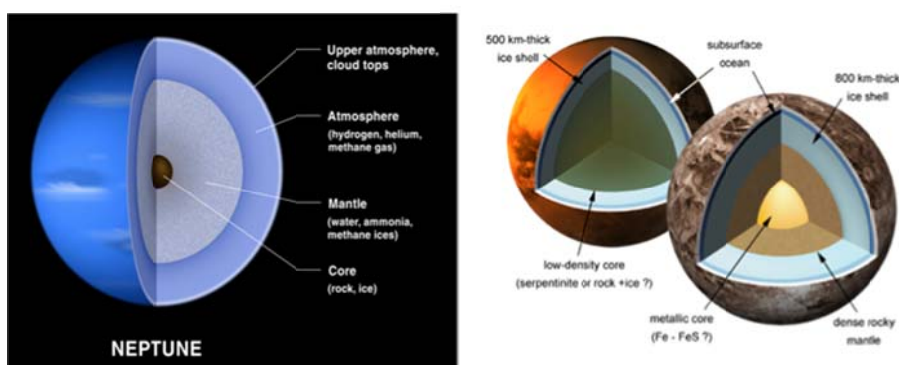


Figure 7: Models of the interior of Neptune and Jupiter's satellites Europa and Ganymede. Water, ammonia, methane and hydrogen under high pressure and temperature are major constituent.

(<http://ircamera.as.arizona.edu/NatSci102/NatSci102/lectures/jupmoon.htm>)

Present investigations of water and aqueous solution under extreme conditions, or in confined reveal the complex behaviour of water are limited by our experimental capabilities [27,34,35]. The study of picoseconds-dynamics, i.e. diffusion, fast relaxation effects, and vibrational dynamics in water and other simple molecular systems under extreme conditions is crucial for a variety of scientific issues spanning most of natural sciences. A few examples; The diffusion of water at pressures of a few GPa's and hundreds of K, typical of the transition zone of the Earth's mantle, has strong incidence on the processes governing volcanic eruptions and intermediate-depth seismicity. Hydrogen diffusion in porous systems and in metals under pressure is fundamental in problems relating to environment, hydrogen storage, and material functionality. Information on molecular re-orientation and hydrogen

delocalization and diffusion in solid water and ammonia under pressures of GPa's and thousands K is essential in order to interpret observations and develop models of planetary interiors and eventually characterize new exotic properties, as the predicted plasticity and superionicity of water and ammonia. The study of the dynamical destabilisation of high-pressure methane clathrates, largely found in the outer solar system (comets, satellites of the gas giant planets, Mars), could clarify methane punctual abundance detected by spatial probes on Titan or Mars.

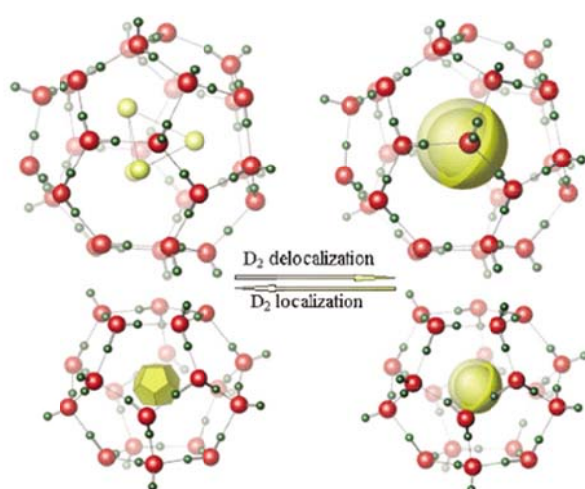


Figure 8 : Structural view of the thermal variation of the D<sub>2</sub> distribution in the large (64512 – hexakaidecahedron, top), and small (512–dodecahedron, bottom) cages in deuterium clathrate. Oxygen atoms are shown as red spheres, deuterium framework atoms–green, and guest D<sub>2</sub> molecules–yellow. Below 50 K, the guest D<sub>2</sub> molecules are localized: in the large cage four molecules are oriented to the centers of hexagons yielding a tetrahedral cluster; in the small cage one D<sub>2</sub> molecule is statistically distributed over 20 positions oriented towards the oxygen atoms forming the dodecahedron. With increasing temperature, the D<sub>2</sub> molecule can more freely rotate, yielding a nearly spherical density distribution inside the cages (right).

In this extent, there is a broad scientific community which will be interested in the possibility of extending INS studies at very high pressures, and both fundamental, and applied research in a wide field ranging from planetary interiors to the recovery to ambient conditions of non-equilibrium structures having novel functional properties, will be promoted.

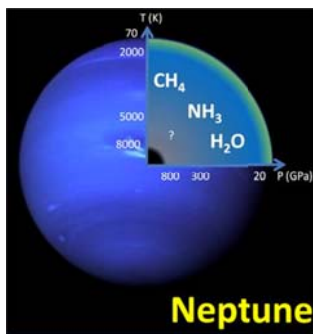


Figure 9: The composition of Neptune.



Figure 10: H-bonded water molecules.

## ii) Experimental Realization of Extreme Pressures and Temperatures for Inelastic Neutron Scattering.

The Mbar pressures that can be achieved for inelastic x-ray scattering unrealistic for inelastic neutron scattering we need to identify a pressure range of interest that may be achievable for inelastic neutron scattering with a wide angular access. A target for high pressure and temperature studies is 30 GPa, the pressure by which all phase transitions in the Earth's upper mantle have occurred. Cambridge University and the Université P & M Curie have developed a Paris-Edinburgh cell with laser access from above and below to achieve high temperatures 2000 K with high pressures for a 65 mm<sup>3</sup> sample space[36]. Increasing the maximum available pressure by a factor just over two would give neutron scattering access to all the structural transformations in the Earth's upper mantle.

An alternative approach to using Paris-Edinburgh cells is using diamond anvil cells. At present using diamond anvil cells for 100-300 K and 25 GPa is readily achieved for powder sample volumes of 20 mm<sup>3</sup>, and can be used for neutron scattering. The current record for successful neutron diffraction in diamond anvil cells now stands at >97 GPa in experiments performed on SNAP at the Spallation Neutron Source, Oak Ridge National Laboratory[37]. Due to thermal insulation, the furnace, electrical contacts etc., a high temperature version is plausible for 1-5 mm<sup>3</sup> sample size for 30 GPa, but to achieve this would require a funded postdoctoral research project with access to neutron beamtime, preferably at a spallation source [38]. Diamond anvil cells for working at high temperature but for samples sizes an order of magnitude smaller are also being developed for use at the Joint Institute for Nuclear Research, with the aim of having a working pressure of 30 GPa[39]. With present development in pressure cells for neutron scattering, by 2020 the technology to produce the necessary high pressure and high temperature cell for CAMEA will exist.

Developing CAMEA for high pressure studies will necessitate that additional components are included into the design of the instrument. To determine the exact pressure that experiments are being carried out at, the lattice parameter of the pressure transferring

medium needs to be determined. To accurately determine the lattice parameter the chopper package needs a 1% high resolution ( $\Delta\lambda/\lambda$ ) mode, a well collimated beam and a neutron diffraction detector. The well collimated beam can be obtained using the WISH beam definition package envisaged for CAMEA. There are two options for a diffraction detector, one is to place a pixelated diffraction detector behind the CAMEA analyzers, a second is to place the detector on the other side of the sample position.

### **iii) User Community**

The geoscience community do not presently use inelastic neutron scattering for studying materials, although there are geoscientists who use neutron diffraction. Any inelastic neutron scattering experiments in geosciences would therefore be from a new user community. The potential for developing a geoscience user community would come from geoscientists with a neutron diffraction, Raman scattering, or x-ray scattering background, or from the experienced inelastic neutron scattering community collaborating with the geoscience community. For example, geoscience studies could be started in collaboration with neutron scatterers that presently study the different phases of types of water under extreme pressures [27,34]. The potential for proof of principal experiments should be investigated with state of the art neutron instrumentation; this would resolve the capabilities of CAMEA for geosciences.

One synergy of research with the geoscience community would be studying the in-situ growth of samples under high pressure and temperature. Geoscience studies under high pressure map out in detailed phase diagrams of materials, these phase diagrams can then be utilized by material scientists to obtain compounds with highly desirable structures, for instance magnetic systems. In-situ studies of the growth of these samples would provide information on the transition from the amorphous phase into single crystals. CAMEA's ability to study diffuse scattering facilitates detailed studies of synthesis phase transitions.

## 4) Concluding Remarks

We have argued the scientific case for CAMEA. In our report we have shown there is a strong existing using neutron scattering community for CAMEA, and that this community already has a strong demand for performing neutron scattering in extreme environments. We have provided a brief outline of how CAMEA advances neutron instrumentation, with the performance gains to be bench marked in neutron instrument simulations. Extreme sample environments presently available or that can be readily achieved have been identified for use with CAMEA. With the presently availability of technology we have outlined the experimental capabilities of CAMEA beyond present neutron instrumentation, and how these capabilities can be utilized for studying magnetism. We have also identified promising avenues for future developments in neutronics that CAMEA would embrace. There is a danger of labelling CAMEA as purely an extreme environment spectrometer but we have clearly identified other areas of research where CAMEA has an advantage, such as time resolved and in-situ studies. CAMEA is an instrument for which there is a clear demand. The capabilities of CAMEA at ESS will be unique in neutron scattering in the world, enabling science that cannot be performed on any other neutron instrumentation.

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